

Kramers degeneracy in a magnetic field and Zeeman spin-orbit coupling in antiferromagnetic conductors

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In this article, I study magnetic response of electron wavefunctions in a commensurate collinear antiferromagnet. I show that, at a special set of momenta, hidden anti-unitary symmetry protects Kramers degeneracy of Bloch eigenstates against a magnetic field, pointing transversely to staggered magnetization. Hence a substantial momentum dependence of the transverse g -factor in the Zeeman term, turning the latter into a spin-orbit coupling, that may be present in materials from chromium to borocarbides, cuprates, pnictides, as well as organic and heavy fermion conductors.

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Antiferromagnetism is a frequent occurrence in materials with interesting electron properties: it is found in elemental [1] and binary [2] solids, in numerous borocarbides [3], in doped insulators such as cuprates [4], in iron pnictides [5], in various organic [6] and heavy fermion [7] compounds. The physics of an antiferromagnetic state in these materials has been a subject of much research.

In this article, I study response of electron states in an antiferromagnet to a weak magnetic field. I concentrate on the simplest case: a commensurate collinear antiferromagnet, shown schematically in Fig. 1, where magnetisation density at any point is parallel or antiparallel to a single fixed direction \mathbf{n} of staggered magnetisation, and changes sign upon primitive translation of the underlying lattice.

In a paramagnet, double degeneracy of single-electron eigenstates is usually attributed to symmetry under time reversal θ – and, indeed, perturbations that break θ (such as ferromagnetism or magnetic field) tend to remove the degeneracy. Yet mere violation of θ does not preclude degeneracy: in a commensurate centrosymmetric Néel antiferromagnet, as in a paramagnet, all Bloch eigenstates enjoy Kramers degeneracy [8] in spite of time reversal being broken in the former, but not in the latter.

In an antiferromagnet, staggered magnetisation sets a special direction \mathbf{n} in electron spin space, making it anisotropic. Magnetic field along \mathbf{n} removes the degeneracy, as it does in a paramagnet. By contrast, in a transverse field, the symmetry remains high enough to protect Kramers degeneracy at a special set of momenta. Generally, in d spatial dimensions, full degeneracy manifold is $(d - 1)$ -dimensional; at its subset, degeneracy is dictated by symmetry. This is in marked contrast with a paramagnet, where arbitrary magnetic field lifts the degeneracy of all Bloch eigenstates.

I show that, at a subset of the degeneracy manifold above, it is a hidden anti-unitary symmetry that protects Kramers degeneracy of Bloch states in a transverse field. The degeneracy gives rise to a peculiar spin-orbit coupling, whose emergence and basic properties, along with the degeneracy itself, are the main result of this work.

Kramers degeneracy of special Bloch states in a transverse field means, that the transverse component g_{\perp} of the electron g -tensor vanishes for such states. Not being identically equal to zero, g_{\perp} must, therefore, carry substantial momentum dependence, and the Zeeman coupling \mathcal{H}_{ZSO} must take the form

$$\mathcal{H}_{ZSO} = -\mu_B [g_{\parallel}(\mathbf{H}_{\parallel} \cdot \boldsymbol{\sigma}) + g_{\perp}(\mathbf{p})(\mathbf{H}_{\perp} \cdot \boldsymbol{\sigma})], \quad (1)$$

where $\mathbf{H}_{\parallel} = (\mathbf{H} \cdot \mathbf{n})\mathbf{n}$ and $\mathbf{H}_{\perp} = \mathbf{H} - \mathbf{H}_{\parallel}$ are the longitudinal and the transverse components of the magnetic field with respect to unit vector \mathbf{n} of staggered magnetisation, μ_B is the Bohr magneton, while g_{\parallel} and $g_{\perp}(\mathbf{p})$ are the longitudinal and the transverse components of the g -tensor.

This very momentum dependence of $g_{\perp}(\mathbf{p})$ turns the common Zeeman coupling into a Zeeman spin-orbit interaction \mathcal{H}_{ZSO} (1), whose appearance and key properties are at the focus of this work. Zeeman spin-orbit coupling may manifest itself spectacularly in a number of ways, which will be mentioned below and discussed in detail elsewhere.

Symmetry properties of wave functions in magnetic crystals have been studied by Dimmock and Wheeler [9], who pointed out, among other things, that magnetism not only lifts degeneracies by obviously lowering the symmetry, but also may introduce new ones. This may happen at the magnetic Brillouin zone (MBZ) boundary, under the necessary condition that the magnetic unit cell be larger, than the paramagnetic one [9].

For a Néel antiferromagnet on a square lattice, response of electron states to magnetic field was studied in [10] by symmetry analysis, and in [11] within a weak coupling model. The present work revisits [10], extends it to an arbitrary crystal symmetry and shows, that the picture is more rich than envisaged by the authors. At the same time, the present work extends [9] by allowing for external magnetic field – to show how, at special momenta, Kramers degeneracy may persist even in a transverse magnetic field.

Antiferromagnetic order couples to the electron spin $\boldsymbol{\sigma}$ via exchange term $(\boldsymbol{\Delta}_r \cdot \boldsymbol{\sigma})$, where $\boldsymbol{\Delta}_r$ is proportional to

the average magnetisation density at point \mathbf{r} . Nonzero $\Delta_{\mathbf{r}}$ changes sign under time reversal θ , and removes the symmetry under primitive translations $\mathbf{T}_{\mathbf{a}}$, thus reducing the symmetry with respect to that of paramagnetic state. In a doubly commensurate collinear antiferromagnet, $\Delta_{\mathbf{r}}$ changes sign upon $\mathbf{T}_{\mathbf{a}}$: $\Delta_{\mathbf{r}+\mathbf{a}} = -\Delta_{\mathbf{r}}$, while $\mathbf{T}_{\mathbf{a}}^2$ leaves $\Delta_{\mathbf{r}}$ intact: $\Delta_{\mathbf{r}+2\mathbf{a}} = \Delta_{\mathbf{r}}$. Even though neither θ nor $\mathbf{T}_{\mathbf{a}}$ remain a symmetry, their product $\theta\mathbf{T}_{\mathbf{a}}$ does (see Fig. 1). In a system with inversion center, so does $\theta\mathbf{T}_{\mathbf{a}}\mathcal{I}$, where \mathcal{I} is inversion.

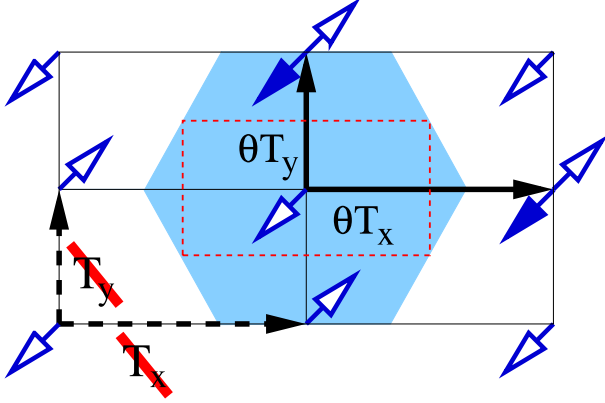


FIG. 1: (color online). Doubly commensurate collinear antiferromagnet on a simple rectangular lattice. In the absence of magnetism, time reversal θ and primitive translations \mathbf{T}_x and \mathbf{T}_y , shown by dashed arrows, are symmetry operations. In the antiferromagnetic state, neither of the three remains a symmetry, but the products $\theta\mathbf{T}_x$ and $\theta\mathbf{T}_y$, shown by solid arrows, do, as illustrated by filled spin arrows. Small dashed rectangle at the center is the Wigner-Seitz cell boundary in the paramagnetic state, while the shaded hexagon is its antiferromagnetic counterpart. Notice that neither of the point group operations interchanges the two sublattices, hence any point symmetry of the lattice, including inversion \mathcal{I} , remains a symmetry of the antiferromagnetic state.

Combined anti-unitary symmetry $\theta\mathbf{T}_{\mathbf{a}}\mathcal{I}$ induces Kramers degeneracy [8]: If $|\mathbf{p}\rangle$ is a Bloch eigenstate at momentum \mathbf{p} , then $\theta\mathbf{T}_{\mathbf{a}}\mathcal{I}|\mathbf{p}\rangle$ is degenerate with $|\mathbf{p}\rangle$. Since θ and \mathcal{I} both invert the momentum, both $|\mathbf{p}\rangle$ and $\theta\mathbf{T}_{\mathbf{a}}\mathcal{I}|\mathbf{p}\rangle$ carry the same momentum label \mathbf{p} . At the same time, $|\mathbf{p}\rangle$ and $\theta\mathbf{T}_{\mathbf{a}}\mathcal{I}|\mathbf{p}\rangle$ are orthogonal: recalling that $(\mathbf{T}_{\mathbf{a}}\mathcal{I})^2 = -\theta^2 = 1$, one finds [8]

$$\langle \mathbf{p} | \theta\mathbf{T}_{\mathbf{a}}\mathcal{I} | \mathbf{p} \rangle = -\langle \mathbf{p} | \theta\mathbf{T}_{\mathbf{a}}\mathcal{I} | \mathbf{p} \rangle. \quad (2)$$

Thus, in spite of broken time reversal symmetry, in a centrosymmetric commensurate Néel antiferromagnet all Bloch states retain Kramers degeneracy.

Generally, magnetic field \mathbf{H} lifts this degeneracy. However, in a purely transverse field, hidden anti-unitary symmetry may protect the degeneracy at a special set of points in the Brillouin zone, as I show below.

In a commensurate collinear antiferromagnet in magnetic field \mathbf{H} , electron Hamiltonian has the form

$$\mathcal{H} = \mathcal{H}_0 + (\Delta_{\mathbf{r}} \cdot \boldsymbol{\sigma}) - (\mathbf{H} \cdot \boldsymbol{\sigma}), \quad (3)$$

where ‘paramagnetic’ part \mathcal{H}_0 is invariant under independent action of $\mathbf{T}_{\mathbf{a}}$ and θ , and $g\mu_B$ is set to unity. In the absence of the field, all Bloch eigenstates of Hamiltonian (3) enjoy Kramers degeneracy by virtue of Eqn. (2).

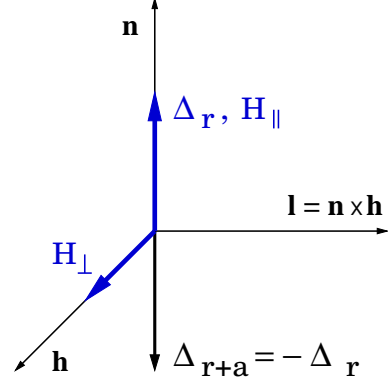


FIG. 2: (color online). Relative orientation of $\Delta_{\mathbf{r}}$, $\Delta_{\mathbf{r}+\mathbf{a}}$, \mathbf{H}_{\parallel} and \mathbf{H}_{\perp} . Notice that θ flips both $\Delta_{\mathbf{r}}$ and \mathbf{H} , while $\mathbf{T}_{\mathbf{a}}$ leaves \mathbf{H} intact, but inverts $\Delta_{\mathbf{r}}$.

Consider symmetries of Hamiltonian (3), involving a combination of an elementary translation $\mathbf{T}_{\mathbf{a}}$, time reversal θ , or a spin rotation $\mathbf{U}_{\mathbf{m}}(\phi)$ around axis \mathbf{m} by angle ϕ . The relative orientation of $\Delta_{\mathbf{r}}$, \mathbf{H}_{\parallel} and \mathbf{H}_{\perp} is shown in Fig. 2.

Transverse field \mathbf{H}_{\perp} breaks the symmetries $\mathbf{U}_{\mathbf{n}}(\phi)$ and $\mathbf{T}_{\mathbf{a}}\theta$ (both change \mathbf{H}_{\perp}), but preserves $\mathbf{U}_{\mathbf{n}}(\pi)\theta\mathbf{T}_{\mathbf{a}}$, their combination at $\phi = \pi$. Acting on the exact Bloch state $|\mathbf{p}\rangle$ at momentum \mathbf{p} , this combined anti-unitary operator creates a degenerate partner eigenstate $\mathbf{U}_{\mathbf{n}}(\pi)\theta\mathbf{T}_{\mathbf{a}}|\mathbf{p}\rangle$, which is orthogonal to $|\mathbf{p}\rangle$ everywhere in the Brillouin zone, unless \mathbf{p} belongs to a paramagnetic Brillouin zone boundary:

$$\langle \mathbf{p} | \mathbf{U}_{\mathbf{n}}(\pi)\theta\mathbf{T}_{\mathbf{a}} | \mathbf{p} \rangle = e^{-2i\mathbf{p}\cdot\mathbf{a}} \langle \mathbf{p} | \mathbf{U}_{\mathbf{n}}(\pi)\theta\mathbf{T}_{\mathbf{a}} | \mathbf{p} \rangle. \quad (4)$$

Equation (4) can be derived analogously to Eqn. (2) as soon as one observes, that $[\mathbf{U}_{\mathbf{n}}(\pi)\theta\mathbf{T}_{\mathbf{a}}]^2 = \mathbf{T}_{\mathbf{a}}^2$.

Notice, however, that eigenstate $\mathbf{U}_{\mathbf{n}}(\pi)\theta\mathbf{T}_{\mathbf{a}}|\mathbf{p}\rangle$ carries momentum label $-\mathbf{p}$ rather than \mathbf{p} . Generally, these two momenta are different. However, an important exception takes place at the magnetic Brillouin zone boundary, if there is a unitary symmetry \mathcal{U} , transforming $-\mathbf{p}$ into a momentum, equivalent to \mathbf{p} modulo reciprocal lattice vector \mathbf{Q} of the antiferromagnetic state [9]:

$$-\mathcal{U}\mathbf{p} = \mathbf{p} + \mathbf{Q}. \quad (5)$$

In this case, eigenstate $\mathcal{U}\mathbf{U}_{\mathbf{n}}(\pi)\theta\mathbf{T}_{\mathbf{a}}|\mathbf{p}\rangle$ carries momentum label $\mathbf{p} + \mathbf{Q} \equiv \mathbf{p}$, is degenerate with $|\mathbf{p}\rangle$ and orthog-

onal to it, thus explicitly demonstrating Kramers degeneracy at momentum \mathbf{p} in a transverse field. In the simplest case, as in Fig. 3 below, \mathcal{U} is the unity operator.

Additional insight into the locus of states, whose degeneracy persists in a transverse magnetic field, is afforded by weak-coupling Hamiltonian of a single electron in a doubly commensurate collinear antiferromagnet. Let \mathbf{Q} be the antiferromagnetic ordering wave vector (see the examples below); $\Delta_{\mathbf{r}}$ creates a matrix element $(\Delta \cdot \sigma)$ between the Bloch states at momenta \mathbf{p} and $\mathbf{p} + \mathbf{Q}$; for simplicity, I neglect its possible dependence on \mathbf{p} . In magnetic field \mathbf{H} , and at weak coupling, Hamiltonian (3) takes the form [11]

$$\mathcal{H} = \begin{bmatrix} \epsilon_{\mathbf{p}} - (\mathbf{H} \cdot \sigma) & (\Delta \cdot \sigma) \\ (\Delta \cdot \sigma) & \epsilon_{\mathbf{p}+\mathbf{Q}} - (\mathbf{H} \cdot \sigma) \end{bmatrix}, \quad (6)$$

where $\epsilon_{\mathbf{p}}$ and $\epsilon_{\mathbf{p}+\mathbf{Q}}$ are single-particle energies of \mathcal{H}_0 in (3) at momenta \mathbf{p} and $\mathbf{p} + \mathbf{Q}$.

In a purely transverse field \mathbf{H}_{\perp} , the spectrum of this Hamiltonian is simply

$$\mathcal{E}_{\mathbf{p}} = \eta_{\mathbf{p}} \pm \sqrt{\Delta^2 + [\zeta_{\mathbf{p}} \mp (\mathbf{H}_{\perp} \cdot \sigma)]^2}, \quad (7)$$

where $\eta_{\mathbf{p}} \equiv \frac{\epsilon_{\mathbf{p}} + \epsilon_{\mathbf{p}+\mathbf{Q}}}{2}$, and $\zeta_{\mathbf{p}} \equiv \frac{\epsilon_{\mathbf{p}} - \epsilon_{\mathbf{p}+\mathbf{Q}}}{2}$. Equation (7) illustrates several points. Firstly, at half-filling, a gap of size 2Δ opens at the chemical potential. Secondly, in the absence of magnetic field, each eigenstate is indeed doubly degenerate, in agreement with the arguments, encapsulated in Eqn. (2). Finally, Eqn. (7) shows, that the degeneracy persists in a transverse field (and, therefore, $g_{\perp}(\mathbf{p})$ in Eqn. (1) vanishes) whenever $\zeta_{\mathbf{p}} = 0$. Barring a special situation, this equation defines a surface in three dimensions, a line in two, and a set of points in one. Furthermore, as shown above, this manifold must contain all points, satisfying Eqn. (5).

Notice that transverse magnetic field not only introduces the last term in Hamiltonian (3), but also tilts the sublattices. However, the resulting magnetisation has the same symmetry as the field, and thus does not remove the degeneracy.

Consider examples. In one dimension, magnetic Brillouin zone boundary reduces to two points $\mathbf{p} = \pm \frac{\pi}{2a}$, which in fact coincide modulo antiferromagnetic wave vector $\mathbf{Q} = \frac{\pi}{a}$, that is also the reciprocal lattice vector of the antiferromagnetic state (see Fig. 3). In terms of the general condition (5), this is the simplest case: $\mathcal{U} = \mathbf{1}$.

As a result, at $\mathbf{p} = \pm \frac{\pi}{2a}$, the two exact Bloch states in a transverse field, $|\mathbf{p}\rangle$ and $\theta \mathbf{T}_{\mathbf{a}} \mathbf{U}_{\mathbf{n}}(\pi) |\mathbf{p}\rangle$, correspond to the *same* momentum \mathbf{p} , and are degenerate by virtue of $\theta \mathbf{T}_{\mathbf{a}} \mathbf{U}_{\mathbf{n}}(\pi)$ being a symmetry. Equation (4) guarantees their orthogonality, thus protecting Kramers degeneracy at momentum $\mathbf{p} = \pm \frac{\pi}{2a}$ against transverse magnetic field.

Now, consider a two-dimensional antiferromagnet of simple rectangular symmetry, with the ordering wave

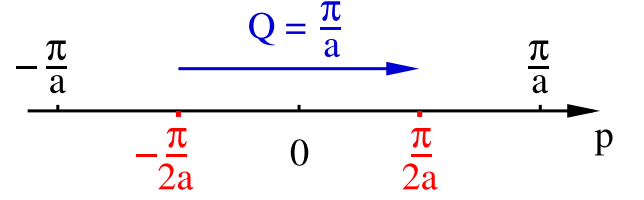


FIG. 3: (color online). The paramagnetic ($\mathbf{p} = \pm \frac{\pi}{a}$), and the antiferromagnetic ($\mathbf{p} = \pm \frac{\pi}{2a}$) Brillouin zone boundaries of a one-dimensional Néel antiferromagnet. In the antiferromagnetic state, the two points $\mathbf{p} = \pm \frac{\pi}{2a}$ are identical modulo the antiferromagnetic reciprocal lattice vector $\mathbf{Q} = \frac{\pi}{a}$. At these two points, anti-unitary symmetry $\mathbf{U}_{\mathbf{n}}(\pi) \mathbf{T}_{\mathbf{a}} \theta$ protects Kramers degeneracy against transverse magnetic field.

vector $\mathbf{Q} = (\pi, \pi)$, as shown in Fig.1. In a transverse magnetic field, degeneracy persists at a line in the Brillouin zone, by virtue of Eqn. (7). I will show that, in the rectangular case, the degeneracy line must contain point Σ (i.e. the star of point $\mathbf{p} = \mathbf{Q}/2$) at the center of the magnetic Brillouin zone boundary (see Fig. 4(a)). Consider a Bloch state $|\mathbf{p}\rangle$ at momentum \mathbf{p} in a trans-

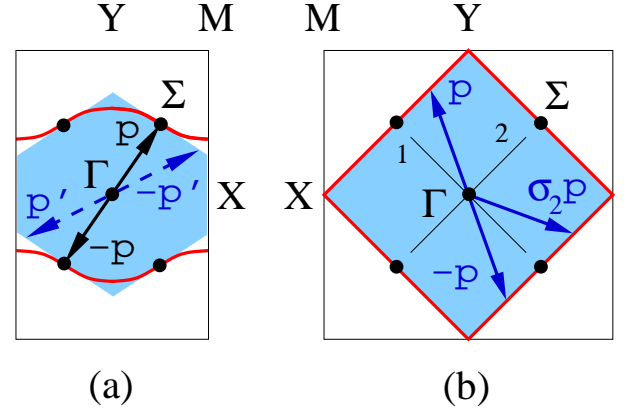


FIG. 4: (color online). Geometry of the problem. (a) The Brillouin zone for a simple rectangular lattice (the rectangle), and its antiferromagnetic counterpart (MBZ, shaded hexagon). Thick curve (red online), passing through point Σ , shows a typical degeneracy line $g_{\perp}(\mathbf{p}) = 0$. At the MBZ boundary, only momentum \mathbf{p} at point Σ is equivalent to $-\mathbf{p}$ modulo the reciprocal lattice vector of the antiferromagnetic state. For a generic \mathbf{p}' , shown by the dashed arrow, this is no longer true. (b) The Brillouin zone of a simple square lattice and its antiferromagnetic counterpart (shaded diagonal square). The degeneracy line must contain the entire MBZ boundary, shown in red online.

verse field. As discussed above, eigenstate $\theta \mathbf{T}_{\mathbf{a}} \mathbf{U}_{\mathbf{n}}(\pi) |\mathbf{p}\rangle$ at momentum $-\mathbf{p}$ is degenerate with $|\mathbf{p}\rangle$ and, according to Eqn. (4), must be orthogonal to it unless $(\mathbf{p} \cdot \mathbf{a})$ is an integer multiple of π . At points Σ (the star of $\mathbf{p} = \mathbf{Q}/2$), X, and Y, momenta \mathbf{p} and $-\mathbf{p}$ coincide modulo a recip-

rocal lattice vector of the antiferromagnetic state. However, at points X and Y (as well as at the entire vertical segment of the MBZ boundary in Fig. 4(a)), $(\mathbf{p} \cdot \mathbf{a})$ is an integer multiple of π ; hence $|\mathbf{p}\rangle$ and $\theta \mathbf{T}_a \mathbf{U}_n(\pi)|\mathbf{p}\rangle$ are not obliged to be orthogonal there as per Eqn. (4). Thus, Σ is the only point at the MBZ boundary, where the two degenerate states $|\mathbf{p}\rangle$ and $\theta \mathbf{T}_a \mathbf{U}_n(\pi)|\mathbf{p}\rangle$ are orthogonal and correspond to the same momentum. Dashed arrows in figure 4(a) show, that, for a generic point \mathbf{p}' at the MBZ boundary, no symmetry operation relates $-\mathbf{p}'$ to a vector, equivalent to \mathbf{p}' . Hence it is only at point Σ , that the symmetry protects Kramers degeneracy against transverse magnetic field. As in the one-dimensional example above, in terms of Eqn. (5) this corresponds to the simplest case of $\mathcal{U} = \mathbf{1}$.

Promotion from rectangular to square symmetry brings along invariance under reflections $\sigma_{1,2}$ in either of the two diagonal axes 1 and 2, passing through point Γ in Fig. 4(b). As a result, eigenstate $\sigma_1 \theta \mathbf{T}_a \mathbf{U}_n(\pi)|\mathbf{p}\rangle$ at momentum $\sigma_2 \mathbf{p}$ (Fig. 4(b)) is also degenerate with $|\mathbf{p}\rangle$ and orthogonal to it, as one can show analogously to the examples above. In terms of general condition (5), this means $\mathcal{U} = \sigma_{1,2}$.

For momentum \mathbf{p} at the MBZ boundary in Fig. 4(b), \mathbf{p} and $\sigma_2 \mathbf{p}$ differ by a reciprocal lattice vector and thus coincide. Hence, for a square-symmetry lattice in a transverse field, Kramers degeneracy is protected by symmetry at the entire MBZ boundary, as shown in Fig. 4(b).

Degeneracy of special Bloch states in a transverse field hinges only on the symmetry of the antiferromagnetic state, and thus holds equally in a strongly correlated or a weakly coupled material – provided long-range antiferromagnetic order and well-defined electron quasiparticles. Under these conditions, quantum fluctuations of the antiferromagnetic order primarily renormalize the sublattice magnetisation, but leave intact the degeneracy of special electron states in a transverse field – certainly in the leading order in fluctuations.

Now, $g_\perp(\mathbf{p})$ can be expanded in a vicinity of the degeneracy line $g_\perp(\mathbf{p}) = 0$. With the exception of higher-symmetry points, such as point X in Fig. 4(b), the leading term of the expansion is linear in momentum deviation $\delta \mathbf{p}$ from the degeneracy line:

$$g_\perp(\mathbf{p}) \approx \frac{\boldsymbol{\Xi}_\mathbf{p} \cdot \delta \mathbf{p}}{\hbar}, \quad (8)$$

where $\boldsymbol{\Xi}_\mathbf{p}/\hbar$ is momentum gradient of $g_\perp(\mathbf{p})$ at point \mathbf{p} on the degeneracy line. Inversion symmetry requires, that $\boldsymbol{\Xi}_\mathbf{p}$ be a pseudo-vector and change sign upon inversion, and Eqn. (7) shows, that $\boldsymbol{\Xi}_\mathbf{p}$ is of the order of the antiferromagnetic coherence length $\xi \sim \frac{\hbar v_F}{\Delta}$.

Zeeman spin-orbit coupling (1) induces a number of

interesting effects. For instance, substantial momentum dependence of $g_\perp(\mathbf{p})$ means, that the Electron Spin Resonance (ESR) frequency of a carrier in a vicinity of the degeneracy line varies along the quasiclassical trajectory. In a weakly doped antiferromagnetic insulator, this means inherent broadening of the ESR line with doping and, eventually, loss of the ESR signal. In fact, this may well be the reason behind the long-known ‘ESR silence’ [12] of the cuprates. Suppression of transverse Pauli susceptibility is another simple consequence of vanishing $g_\perp(\mathbf{p})$.

Finally, momentum dependence of $g_\perp(\mathbf{p})$ allows excitation of spin flip transitions by AC *electric* rather than magnetic field [13] – a vivid effect of great promise for controlled spin manipulation, so much sought after in spin electronics. Its absorption matrix elements are defined by $\Xi_\mathbf{p} \sim \xi$ of Eqn. (8), and exceed those of ESR at least by two orders of magnitude. According to Eqn. (8), resonance absorption in this phenomenon shows a non-trivial dependence on the orientation of the AC electric field with respect to the crystal axes, and on the orientation of the DC magnetic field with respect to staggered magnetisation.

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